Regression Technique for Determining Temperature Profiles in the Upper Stratosphere From Satellite-Measured Radiances

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ABSTRACT—This paper describes a statistical regression technique for specifying the vertical temperature profile above 10 mb from satellite radiances simulated for the Satellite Infrared Spectrometer B (SIRS B) instrument when the temperature profile up to 10 mb is known. Sensitivity of the radiance information to temperature at the high atmospheric levels is attained by subtracting, from the total radiance, that part of the radiance emanating from the known temperature profile below 10 mb. The remainder is that portion of the radiance representative of the temperature profile above 10 mb. Statistics are derived using a sample of 50 carefully selected temperature profiles representative of worldwide atmospheric conditions above 30 km during all times of the year. Regression

equations are developed relating temperature at 10 pressure levels between 10 and 0.5 mb to a set of predictors [temperature at 50, 30, and 10 mb and radiance information derived from SIRS B channels 7 (679.8 cm⁻¹) and 8 (668.7 cm⁻¹)]. For an independent data set, root-mean-square errors in specification ranged from 2.1°C at 9 mb to 8.8°C at 0.5 mb, with the shapes of all profiles very well distinguished. Regression-specified temperatures above 10 mb are then used as first guess in simulated retrievals of complete atmospheric temperature profiles. These regression results are shown to significantly increase the accuracy of temperature retrievals at tropospheric as well as stratospheric levels over those retrievals derived using a climatological first guess.

1. INTRODUCTION

In recent years, there has been great interest in the problem of deriving the earth's atmospheric thermal structure from satellite radiation observations. Since the inverse solution to the radiative transfer equation using any finite number of independent radiance measurements is, in general, not unique, some constraints are usually placed on the solution in accordance with known properties of the atmosphere. Recent studies of the temperature inversion problem by Smith et al. (1970), Rodgers (1970), Smith and Fleming (1972), and others have stressed that an optimum solution should be based on the use of statistical relationships. Usually, a "first-guess" profile is adjusted to satisfy observed radiances in conformity with an algorithm (such as maximum probability and minimum variance) and multiple regression relationships between the radiance observations and the atmospheric thermal state. Additional information may also be used to provide the best possible first-guess profile. For the retrieval of temperature profiles for dynamical forecasting at the National Meteorological Center (NMC), Smith et al. (1972) use a first-guess profile up to 10 mb derived from analyses or forecasts of temperature obtained principally from radiosonde information. Above 10 mb, a climatological first guess is used. It has been shown by Smith et al. (1972) that generally, for clear sky conditions at levels below 10 mb, temperature profiles can be specified

accurately (i.e., temperature errors less than $\pm 3^{\circ}$ C) regardless of the representativeness of the first guess. At levels higher in the atmosphere, there is an increasing dependence of the solution on the first guess. We will show in section 4 of this paper that, under certain circumstances (e.g., strongly anomalous stratospheric conditions), the use of a climatological first-guess profile may lead to considerable error in the temperatures retrieved.

The work of Quiroz (1971) has shown that sufficient information is available in the Satellite Infrared Spectrometer A (SIRS A) stratospheric channels to specify temperature changes at 30–50 km during stratospheric warmings. His study was restricted to the stratospheric warming phenomenon, but it has led us to inquire whether sufficient information is available in measurements from SIRS-type instruments to specify the stratospheric temperature structure in the general case.

This paper describes a statistical regression technique for specifying the vertical temperature profile for a wide range of atmospheric conditions between 10 and 0.5 mb (approx. 30–55 km) when the temperature profile below 10 mb is known, using radiances simulated for the SIRS B instrument. The application of this technique to "real-time" temperature retrievals could lead to significantly improved temperature specification (especially during times of anomalous stratospheric conditions) not only in the upper stratosphere but also in the lower stratosphere and upper troposphere.

2. DATA

The basic data set consisted of a number of profiles selected so as to be representative of the largest possible variety in shape. Several thousand temperature soundings from the World Data Center A (1964-68) were scrutinized. Fifty profiles were chosen using the criterion that the shape of each sounding selected for the sample should appear significantly different above 30 km from the others chosen. Most of the profiles were chosen from northern latitude locations such as Fort Greely, Alaska, Fort Churchill, Canada, West Geirinish, Scotland, Heiss Island, U.S.S.R., and Thule, Greenland, because there is maximum variability in the stratosphere at high latitudes and, therefore, a wide variety of shapes in the vertical temperature profile is possible. Lower latitude soundings have shapes that are similar to one another, except that an entire profile may be warmer or colder depending on latitude and season. It is for this reason that a relatively small number of profiles from low latitudes are able to represent conditions there. Soundings were chosen from lower latitude stations at Point Mugu, Calif., White Sands, N. Mex., Cape Kennedy, Fla., Fort Sherman, C.Z., and Ascension Island.

For each of the 50 soundings chosen for the dependent sample, the full observed temperature profile was used. This profile was comprised of a radiosonde profile from the surface to approximately 20 km and a rocketsonde profile from 20 km to approximately 60 km. In some cases, the rocketsonde profile extended up to 80 km, but when it didn't, a climatological profile taken from the U.S. Standard Atmosphere Supplements (COESA 1966) was used to augment the observed profile above its maximum level. Each of the soundings was then put in the form of temperature versus pressure, and a computer program interpolated the profile to each of 100 pressure levels at $p^{2/7}$ intervals between 1000 and 0.01 mb.

The 50 temperature profiles were then used in simulating the radiance information that the SIRS B instrument would measure when observing a clear atmospheric column having the given vertical temperature configuration (Smith et. al. 1972). The transmittance weighting functions $(d\tau/dx$, where $x=p^{2/7}$) used are shown in figure 1. For the two most opaque channels [channels 8 (668.7 cm⁻¹) and 7(679.8 cm⁻¹)] the contributions to the radiance from the atmospheric column up to 10 mb [henceforth referred to as I8L (lower) and I7L] and from the portion of the column above 10 mb [I8U (upper), I7U] were computed separately, in addition to the total radiance. Random noise of the SIRS instrument was simulated by adding to the computed radiances a random error. The magnitudes of the errors in each of the 50 sample cases were obtained by a random number generator which operated so that the root-mean-square (rms) value of the errors was $0.25 \times 10^{-7} \text{J} \cdot \text{cm}^{-2} \cdot \text{s}^{-1} \cdot (\text{ster})^{-1} \cdot \text{cm}^{-1})^{-1}$.

3. REGRESSION ANALYSIS

Regression equations were derived relating the temperatures at levels above 10 mb to temperatures at levels

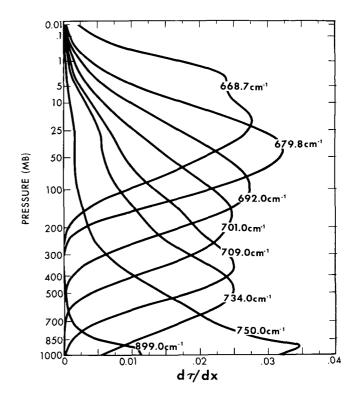


FIGURE 1.—Derivative of transmittance (τ) with respect to $x(p) = p^{2/7}$ for SIRS B.

below 10 mb and the simulated radiance information. The temperatures at 10 pressure levels, 9.08, 7.95, 6.92, 5.99, 5.16, 3.74, 2.63, 1.77, 1.14, and 0.52 mb, were chosen as the predictands. [The pressure level interval was taken to correspond with Smith et al. (1972).] The six predictors used for the specification of temperatures above 10 mb were the temperatures at 50, 30, and 10 mb (T50, T30, T10) and three derived radiance quantities (I8U, I7U, I8U/I8). These independent variables were chosen because a preliminary study indicated that they were well correlated with temperatures at the 5- and 2-mb levels and they could be conveniently obtained at the time of operational derivation of retrievals at the NMC as discussed in section 5.

Multiple regression coefficients were computed for each predictand from the dependent sample of 50 profiles. The form of the regression equations is given by

$$T(p) = A_0 + A_1 T50 + A_2 T30 + A_3 T10 + A_4 I8U + A_5 I7U + A_6 I8U/I8$$

where T(p) is the temperature at any of the 10 pressure levels and A_0 through A_6 are the derived coefficients (table 1).

To assess the contribution of each independent variable to the specified temperature at a particular level, one must take into account the magnitudes of the variables themselves (table 1). Also of interest is the variation of the coefficients with decreasing pressure. For example, the coefficients for the temperature at 10 mb go through a regular change from maximum positive at 9.08 mb to maximum negative at 0.52 mb. This type of variation with height is also seen in the other coefficients.

Table 1.—Dependent sample statistics (°K)

Predictor Range		T50 195~237	T30	T10	<i>I8I</i> 16–38*	17U 6-14*	I8 U/I8 0. 34-0. 62	Rms error (°K)	Explained
Coefficient	Ao	A_1	A_2	A_3	A4	A_{5}	As		· · · · · · · · · · · · · · · · · · ·
Predictand								with 6 predictors	
T(0.52)	-61.9287	0. 7344	0, 6976	0. 4333	-0, 7327	—1. 0667	286. 0215 (20. 5) †	9. 6	37. 9
T(1.14)	-30. 7677	0. 5258	0, 3974	0. 1988	4. 3082 (67. 0)	-8.9233	209. 9237	7.7	83. 4
T(1.77)	92. 1008	0. 7370	0, 2967	0. 1584	2.9169 (82.8)	-4. 8825	255. 8382	5. 5	92.4
T(2.63)	123. 1668	0. 3023	-0.0484	-0.1604	1.8716 (92.2)	2.0661	73, 6523	4. 3	93. 9
T(3.74)	184. 3306	0. 3271	-0.3004	-0. 1542	0.6492 (85.7)	6, 6797	12, 4852	5. 7	88.8
T(5.16)	102. 2657	-0.0290	0.0472	0. 2994	0. 8829	6.7870 (90.5)	44. 0873	4.0	92. 7
T (5.9)	113, 6232	—0. 1741	0, 0539	0.4648	-0.9730	6. 2563 (85. 3)	15, 4026	3. 3	94.3
T(6.92)	121. 8102	-0. 2427	-0.0417	. 6687 (83. 2)	-0.7434	5. 1319	-18, 1930	2.6	96. 3
T(7.95)	59. 8739	-0. 1286	0, 0450	. 7436 (91. 0)	0. 7751	3, 7424	8, 9789	2.1	97. 3
T(9.08)	69. 9282	0. 1035	-0.1061	. 8900 (95, 9)	0.0080	1.8688	-32, 1918	1.7	98. 2

[†]Parentheses indicate percent of variance accounted for by most significant predictor.
*See text for radiance units

Table 2.—Independent Sample Statistics (°K)

Predictand	Range	Mean error	Mean abso- lute error	Rms error	Maximum error
T(0.52)	220-298	2. 0	8. 9	11. 1	27
T(1.14)	216-294	0. 5	6. 1	8. 2	24
T(1.77)	214 - 299	-0.2	5. 2	7. 2	25
T(2.63)	211-292	0. 7	4. 7	5. 9	16
T(3.74)	211-300	0. 0	5. 0	6. 7	23
T(5.16)	208-288	-0.2	4. 0	6. 2	27
T(5.99) .	205-271	0. 2	3. 3	4.8	19
T(6.92)	198-256	0. 7	2. 4	3. 0	9
T(7.95)	193-247	0. 3	2. 0	2. 4	6
T(9.08)	189-245	0. 7	1. 6	2. 1	5

The regression equations, when applied to the dependent data sample, specified the temperature above 10 mb quite well. More than 90 percent of the variance is explained by the equations from 9.08 to 1.77 mb, with 37 percent explained even at the 0.52-mb level (table 1). The rms error ranges from 1.7°C at the lowest level to 9.6°C at the highest.

To test the applicability of the derived regression equations to any meteorological situation, we gathered an independent sample of data. This sample was comprised of 65 vertical temperature profiles with a large range in values from a broad geographical distribution and for times throughout the year. The independent data were processed in the same way as the dependent data discussed in section 2. Temperatures at levels above 10 mb were specified by applying the regression equations to the independent data sample. The results are shown in table 2. Root-mean-square errors in specification range from 2.1°C at 9.08 mb to 11.1°C at 0.52 mb, with the mean error (bias) very close to zero. The wide range of shapes in the independent sample may be seen in figure 2. There is very close agreement between the actual and specified temperature values in curves c-h of figure 2. Curves a and b of figure 2 are two of the worst cases from the independent sample, with errors ranging up to 27°C at the highest level. However, in all of the cases, the shapes of the profiles are very well described.

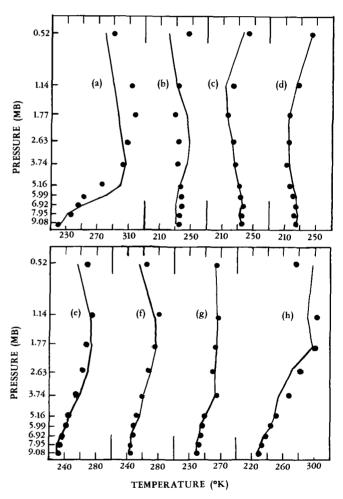


FIGURE 2.—Actual temperature profile (solid lines) and specifications (filled circles) for eight cases in the independent sample: (a) West Geirinish, Scotland, Jan. 1, 1970, (b) Heiss Island, U.S.S.R., Jan. 14, 1970, (c) Fort Greely, Alaska, Dec. 4, 1968, (d) Fort Churchill, Canada, Dec. 9, 1968, (e) Wallops Island, Va., Jan. 15, 1969, (f) Fort Sherman, C.Z., Sept. 22, 1969, (g) Mar Chiquita, Argentina, Jan. 30, 1969, and (h) McMurdo Sound, Antarctica, Sept. 27, 1962.

4. RESULTS USING REGRESSION PROFILE AS FIRST GUESS IN RETRIEVAL SCHEME

The results presented in the previous section are very interesting and could in themselves be very useful. How-

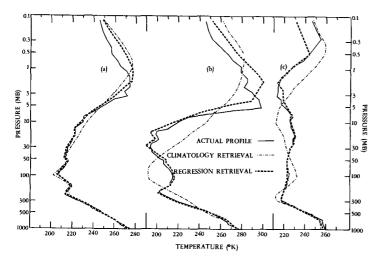


FIGURE 3.—Actual temperature profiles and simulated retrievals for three cases in the independent sample: (a) Wallops Island, Va., Jan. 15, 1969, (b) West Geirinish, Scotland, Jan. 1, 1970, and (c) Fort Churchill, Canada, Dec. 9, 1968.

ever, they assume added significance when applied to the problem of retrieving the complete vertical temperature profile in the troposphere as well as in the stratosphere.

Figure 3 shows a series of simulations derived with the computational methods of Smith et al. (1972) for the retrieval of atmospheric temperature profiles. These simulations are compared with the actual temperature profiles taken from the independent sample discussed in section 3. When retrieved temperature soundings are derived for use in dynamical forecasting at the NMC, the first-guess profiles are constructed from analyses or forecasts of temperature at levels up to 10 mb and climatological values (COESA 1966) above 10 mb.¹

For the retrievals shown by the dash-dot lines, we have used, as the first guess, climatological information above 10 mb and the actual profile below 10 mb. Radiances were calculated for the actual temperature profiles using the transmittance weighting functions of the SIRS B instrument. Random errors in the radiances were introduced as in the previous sections. Curve a of figure 3 shows the type of agreement between the retrieval and the true temperature profile that is attainable using this operational method. Smith et al. (1972) have shown results very similar to this and concluded that in general, for clear sky conditions, temperature profiles can be specified accurately below 10 mb by this method regardless of the representativeness of the first guess. When, however, the first guess is very different from the actual profile above 10 mb, results such as shown by curves b and c of figure 3 could occur. Under the conditions of a strongly anomalous stratospheric thermal state, climatological values would be very different from the true values. In these cases, the effects of the differences in the first guess at levels above

10 mb are seen in the temperature retrievals down to 300 mb. This is due to the reduced weighting in the transmittance weighting functions above 30 mb. Thus, the bulk of the energy, which in curve b of figure 3 is actually due to the large warming at upper stratospheric levels, is incorrectly ascribed to lower levels (near the peak of channels 7 and 8). When the other channels come into play during the retrieval process, compensation occurs, causing the error to be propagated to lower levels. The nature of this compensation/propagation phenomenon is more readily apparent when one considers the actual coefficients of the temperature-retrieval solution instead of the weighting functions themselves. (See fig. 3 of Smith et al. 1972.)

The heavy dashed lines in figure 3 show the results when the first guess below 10 mb is again the actual profile, but the guess above 10 mb is derived using the regression method described in the previous sections. The total radiance is computed as before, but, in addition, the portion of the radiance emanating from the profile below 10 mb (I8L, I7L) is also computed. This radiance contribution from the lower portion is then subtracted from the total radiance (including a random error) to give the portion of the radiance coming from the levels above 10 mb (I7U, I8U). The simulated random error is thus concentrated at the upper levels. These values (17U, 18U, 18U/18) together with the known values of T50, T30, and T10 were used in the regression equations to derive the temperature at the 10 levels from 9.08 to 0.52 mb. The temperature profile above 10 mb was then constructed assuming linear lapse rates between the specified levels. Above 0.5 mb, a climatological profile was used because the retrieval scheme requires specification to 0.01 mb (even though less than 1 percent of the energy in any channel emanates from levels above 0.5 mb). The regression retrievals above 10 mb are hardly distinguishable from the regression first guess (cf. curves a, b, c of fig. 3 with filled circles in fig. 2 profiles e, a, d, respectively) showing that essentially all the information content of the radiances was used in the regression process. The retrieved temperature profiles using these first-guess profiles reproduce the shapes of the true profiles quite well. The errors in the first guess, especially in the extreme cases of warming and cooling (curves b, e, respectively, of fig. 3), caused only slightly incorrect values for the retrieved temperatures from 10 to approximately 30 mb, with virtually no error propagated below that level.

Table 3 shows the mean and standard deviation, σ , of the errors at selected levels for both the climatology and regression retrievals using the independent sample of 65 profiles. The mean errors for the two retrieval methods are not significantly different at any level. However, the standard deviations for the regression retrievals are consistently less than for the climatology retrievals. The small standard deviation of the errors is especially significant below 10 mb, indicating the possibility of using the regression means for operational retrieval of atmospheric temperature profiles.

¹ This method was in use up to Nov. 5, 1971, after which time a modified version of the method herein described has been utilized. The modification involves the use of total measured radiances in channels 8 and 7 (rather than partitioned radiances) to specify, through regression, the first guess above 10 mb.

Table 3.—Retrieval minus actual profile (°K), independent sample

/mls.)	Climatolog	gy retrieval	Regression retrieval		
<i>p</i> (mb)	Mean	σ	Mean	σ	
0. 89	5. 7	12. 8	1. 0	7. 9	
2. 17	1. 2	8. 2	1. 0	5. 8	
3. 15	 0. 7	10. 0	1. 0	6. 7	
5. 16	-2.3	9. 3	0. 8	7. 0	
10. 32	-0.7	9. 7	0. 4	1. 4	
20. 43	-0. 1	7. 4	0. 3	1. 0	
30. 21	0. 1	4. 3	0. 2	0. 6	
50. 56	0. 2	2. 5	0. 0	0.8	
97. 21	-0. 1	7. 1	-0.2	0.8	
98. 99	-0.1	2. 4	0. 1	0. 9	
299. 01	-0.2	3. 3	0. 2	0. 5	

5. CONCLUSIONS

We have demonstrated by simulating radiance measurements for the SIRS B instrument that, for a wide range of atmospheric temperature profiles, the temperature structure between 30 and 55 km may be derived with an expected error of from less than 3°C at 30 km to less than 10°C at 55 km, given the temperature structure in the lower 30 km of the profile and given a consistent and and accurate set of radiance observations.

The importance of these results would be in their application to obtaining complete temperature profiles using actual measured radiances on a real-time basis. Previous investigators have shown that in the altitude region where there is significant weighting for the SIRS instrument—in the troposphere (especially in the absence of clouds) and in the lower stratosphere (during most of the year when the stratosphere is not undergoing strongly anomalous changes)—temperature retrievals of very good representativeness could be obtained. Application of the regression method herein described could almost double the altitude range over which useful temperature retrievals may be obtained and also increase the accuracy of the temperature retrievals at tropospheric levels.

Some cautionary notes are in order, however:

- 1. The sample of rocketsonde temperature profiles chosen in the derivation of the regression equations was assumed to be representative of atmospheric conditions from 30- to 60-km altitudes over the entire world. There has been no indication to date that this assumption is not valid (i.e., we have found no profile that could not be specified acceptably using this set of regression equations). However, it is possible that, over particular geographical regions where we have had no meteorological rocketsonde information, different regression equations would be required.
- 2. The regression equations given in this paper were derived for the SIRS B instrument, which has been designed as a sensor primarily for the troposphere and lower stratosphere. For any other instrument similar to SIRS but with slightly different transmittance weighting functions, it would be relatively easy to derive new regression coefficients useful for that instrument. The procedure could also be adapted for an instrument such as the Selective Chopper Radiometer (SCR) with little difficulty.

- 3. A characteristic of the SIRS B instrument is that the expected error for any of its radiance measurements is less than 0.25×10^{-7} J·cm⁻²·s⁻¹·(ster)⁻¹·(cm⁻¹)⁻¹. The results of this study are dependent on the excellent quality of the instrumental radiance measurements. Any set of measurements with expected errors significantly greater than 0.25×10^{-7} J·cm⁻²·s⁻¹·(ster)⁻¹·(cm⁻¹)⁻¹ could not be used with as much confidence. Because of the nature of the regression method described in this paper, the error would be concentrated in the levels above 10 mb. This error could seriously degrade the representativeness of the temperature profile above 10 mb, but this concentration would be beneficial for the retrieved temperature profile below 10 mb because the error would not be spread out over the entire profile.
- 4. In addition, if the temperature profile below 10 mb (used in the regression equations for specification of upper atmosphere temperature) were in error to any considerable extent (i.e., due to an inaccurate analysis or forecast of temperature at 10 mb or below), the computed radiance contribution from the lower portion (ISL, I7L) would be in error. When this erroneous value is subtracted from the (correct) observed radiance, the contribution of the radiance above 10 mb (ISU, I7U) would be incorrect. This would also result in concentrating the error in the specified temperature above 10 mb
- 5. When the method of regression retrieval described in this paper is used with measurements of a particular instrument, results are highly dependent on a precise knowledge of the transmittance weighting functions of that instrument. Serious error would result if the theoretically derived weighting functions did not precisely coincide with the actual characteristics of the instrument.
- 6. The method used here to derive the temperature profile above 10 mb could possibly be applied at lower levels. Thus, if data were not available at 10 mb, new regression equations could be derived using the 30-mb level (or a lower level) as a base. However, the effect of shifting the base level nearer to the peaks of the weighting functions would have to be evaluated carefully. It would also be possible to use other predictors, such as total radiance (I8, I7), instead of the upper portion radiances (I8U, I7U, I8U/I8) that were used in this study.
- 7. It would have been highly desirable to expand this simulation study by showing results of this method using actual measurements of the SIRS B instrument. However, three difficulties were discovered that, unfortunately, precluded a full and meaningful test. The first problem was an inconsistency between rocketsonde measurements and SIRS B measurements; the satellite measurements exhibited a bias with respect to radiances computed from rocketsonde temperature profiles (Miller and Finger 1972). The second problem was that such a test requires predictors at 50, 30, and 10 mb which, under operational conditions, would be derived from analyzed temperature fields. During the winter period of interest, the NMC objectively analyzed temperature fields at these levels were sometimes considerably in error. One of the contributing factors for this arose from the use of SIRS B retrieval data (using the climatology guess above 10 mb) in these operational analyses. Finally, the overall data coverage was such that only a very small number of cases occurred in which both rocketsonde and satellite observations were available with reasonably small separations in space and time. Although this last problem could have been somewhat circumvented by comparison of SIRS data with the more plentiful radiosonde information for lower levels, the other two problems would have considerably diminished the usefulness of such a test. The above considerations should not detract from the overall significance of the results of the simulation study. To the contrary, they call for concentrated research on the problem areas enumerated.

The impact of the above considerations in terms of the utility of this regression method for operational retrieval of atmospheric temperature profiles from actual measured radiances on a real-time basis is now under active investigation.

The simulation study shows that, given accurate observational values for predictors, the temperature profile above 10 mb can be specified with high reliability; and, consequently, improvement of the retrieved temperature profiles below 10 mb is to be expected. We look forward to the availability of fully suitable data for operational testing.

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